Conventions, Accuracy Metrics, Classification, Regression

Nipun Batra

IIT Gandhinagar

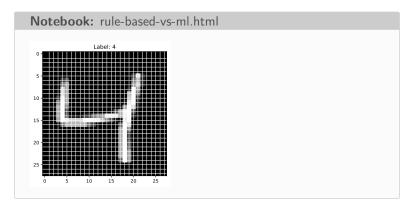
August 1, 2025

Outline

- 1. Introduction to Machine Learning
- 2. Machine Learning Fundamentals
- 3. Classification vs Regression
- 4. Evaluation Metrics
- 5. Advanced Topics

Digit Recognition Problem

Let us work on the digit recognition problem.



Maybe 4 can be thought of as: |+--+| + another vertical |

 The heights of each of the | need to be similar within tolerance

Maybe 4 can be thought of as: |+--+| + another vertical |

 The heights of each of the | need to be similar within tolerance

- The heights of each of the | need to be similar within tolerance
- Each of the | can be slightly slanted. Similarly the horizontal line can be slanted.

- The heights of each of the | need to be similar within tolerance
- Each of the | can be slightly slanted. Similarly the horizontal line can be slanted.

- The heights of each of the | need to be similar within tolerance
- Each of the | can be slightly slanted. Similarly the horizontal line can be slanted.
- There can be some cases of 4 where the first | is at 45 degrees

- The heights of each of the | need to be similar within tolerance
- Each of the | can be slightly slanted. Similarly the horizontal line can be slanted.
- There can be some cases of 4 where the first | is at 45 degrees

- The heights of each of the | need to be similar within tolerance
- Each of the | can be slightly slanted. Similarly the horizontal line can be slanted.
- There can be some cases of 4 where the first | is at 45 degrees
- There can be some cases of 4 where the width of each stroke is different

Pop Quiz: Rule-Based vs ML

Quick Quiz 1

Why is it difficult to write rules for digit recognition?

a) Digits are always the same

Answer: b) Handwriting variations make rule-based approaches extremely complex!

Pop Quiz: Rule-Based vs ML

Quick Quiz 1

Why is it difficult to write rules for digit recognition?

- a) Digits are always the same
- b) Variations in handwriting, rotation, thickness make rules complex

Answer: b) Handwriting variations make rule-based approaches extremely complex!

Pop Quiz: Rule-Based vs ML

Quick Quiz 1

Why is it difficult to write rules for digit recognition?

- a) Digits are always the same
- b) Variations in handwriting, rotation, thickness make rules complex
- c) Rules are faster than ML

Answer: b) Handwriting variations make rule-based approaches extremely complex!

• Size

• Size

• Size

- Size
- Colour

- Size
- Colour

- Size
- Colour
- Texture

Should We Include Sample Numbers?

Answer: Usually no! Sample numbers are typically arbitrary identifiers and not meaningful features. Let us remove it.

Should We Include Sample Numbers?

Answer: Usually no! Sample numbers are typically arbitrary identifiers and not meaningful features. Let us remove it. Let us modify our data table for now.

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad

The training set consists of two parts:

The training set consists of two parts:

The training set consists of two parts:

1. Features (Input Variables)

The training set consists of two parts:

1. Features (Input Variables)

The training set consists of two parts:

- 1. Features (Input Variables)
- 2. Output or Response Variable

Dataset Notation

We call this matrix as \mathcal{D} , containing:

1. Feature matrix $(\mathbf{X} \in \mathbb{R}^{n \times d})$ containing data of n samples each of which is d dimensional.

Dataset Notation

We call this matrix as \mathcal{D} , containing:

- 1. Feature matrix $(\mathbf{X} \in \mathbb{R}^{n \times d})$ containing data of n samples each of which is d dimensional.
- 2. Output vector $(\mathbf{y} \in \mathbb{R}^n)$ containing output variable for n samples.

Dataset Example

```
Example (after encoding): \mathbf{x}_1 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} (Orange=1, Small=0, Smooth=1)
```

Dataset Example

```
Example (after encoding): \mathbf{x}_1 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} (Orange=1, Small=0, Smooth=1)
```

Dataset Example

Example (after encoding):
$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$
 (Orange=1, Small=0, Smooth=1)

• Complete dataset: $\mathcal{D} = \{(\mathbf{x}_i^\top, y_i)\}_{i=1}^n$

Machine Learning Goal

Learn f: Condition = f(colour, size, texture)

Machine Learning Goal

Learn f: Condition = f(colour, size, texture)

Machine Learning Goal

Learn f: Condition = f(colour, size, texture)

1. From Training Dataset

Machine Learning Goal

Learn f: Condition = f(colour, size, texture)

1. From Training Dataset

Machine Learning Goal

Learn f: Condition = f(colour, size, texture)

- 1. From Training Dataset
- 2. To Predict the condition for the Testing set

Colour	Size	Texture	Condition
Orange	Small	Smooth	Good
Red	Small	Rough	Good
Orange	Medium	Smooth	Bad
Yellow	Large	Smooth	Bad
Red	Large	Rough	?
Orange	Large	Rough	?

A: Ideally, no!

A: Ideally, no!

A: Ideally, no!

• Ideally - we want to predict "well" on all possible inputs. But, can we test that?

A: Ideally, no!

• Ideally - we want to predict "well" on all possible inputs. But, can we test that?

A: Ideally, no!

- Ideally we want to predict "well" on all possible inputs. But, can we test that?
- No! Since, the test set is only a sample from all possible inputs.

Training vs Test Sets

Both the training set and the test set are samples drawn from the hidden true distribution (also sometimes called population)

Training vs Test Sets

Both the training set and the test set are samples drawn from the hidden true distribution (also sometimes called population) More discussion later once we study bias and variance

• # People (More people \implies More Energy)

• # People (More people \implies More Energy)

• # People (More people \implies More Energy)

- # People (More people ⇒ More Energy)
- Temperature (Higher Temp. \implies Higher Energy)

- # People (More people ⇒ More Energy)
- Temperature (Higher Temp. ⇒ Higher Energy)

# People	Temp (C)	Energy (kWh)
4000	30	30
4200	30	32
4200	35	40
3000	20	?
1000	45	?

Pop Quiz: Training Data

Quick Quiz 2

What makes a good feature for machine learning?

a) Sample ID numbers

Answer: b) Features should be meaningful and related to what you're predicting!

Pop Quiz: Training Data

Quick Quiz 2

What makes a good feature for machine learning?

- a) Sample ID numbers
- b) Meaningful characteristics that relate to the output

Answer: b) Features should be meaningful and related to what you're predicting!

Pop Quiz: Training Data

Quick Quiz 2

What makes a good feature for machine learning?

- a) Sample ID numbers
- b) Meaningful characteristics that relate to the output
- c) Random numbers

Answer: b) Features should be meaningful and related to what you're predicting!

Classification

Classification

Classification

- Classification
 - Output variable is discrete

- Classification
 - Output variable is discrete

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, \dots, k\}$ where k is number of classes

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, \dots, k\}$ where k is number of classes

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, \dots, k\}$ where k is number of classes
 - Examples Predicting:

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, \dots, k\}$ where k is number of classes
 - Examples Predicting:

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, \dots, k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, \dots, k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, \dots, k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, \dots, k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression
 - Output variable is continuous

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression
 - Output variable is continuous

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression
 - Output variable is continuous
 - \circ i.e. $y_i \in \mathbb{R}$

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression
 - Output variable is continuous
 - \circ i.e. $y_i \in \mathbb{R}$

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression
 - Output variable is continuous
 - i.e. $y_i \in \mathbb{R}$
 - Examples Predicting:

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression
 - Output variable is continuous
 - i.e. $y_i \in \mathbb{R}$
 - Examples Predicting:

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression
 - Output variable is continuous
 - i.e. $y_i \in \mathbb{R}$
 - Examples Predicting:
 - How much energy will campus consume?

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression
 - Output variable is continuous
 - i.e. $y_i \in \mathbb{R}$
 - Examples Predicting:
 - How much energy will campus consume?

- Classification
 - Output variable is discrete
 - i.e. $y_i \in \{1, 2, ..., k\}$ where k is number of classes
 - Examples Predicting:
 - Will I get a loan? (Yes, No)
 - What is the quality of fruit? (Good, Bad)
- Regression
 - Output variable is continuous
 - i.e. $y_i \in \mathbb{R}$
 - Examples Predicting:
 - How much energy will campus consume?
 - How much rainfall will fall?

Pop Quiz: Problem Types

Quick Quiz 3

Predicting house prices is an example of:

a) Classification (discrete output)

Answer: b) Regression - house prices are continuous values!

Pop Quiz: Problem Types

Quick Quiz 3

Predicting house prices is an example of:

- a) Classification (discrete output)
- b) Regression (continuous output)

Answer: b) Regression - house prices are continuous values!

Pop Quiz: Problem Types

Quick Quiz 3

Predicting house prices is an example of:

- a) Classification (discrete output)
- b) Regression (continuous output)
- c) Neither

Answer: b) Regression - house prices are continuous values!

Accuracy Calculation

Accuracy =
$$\frac{|\{i : y_i = \hat{y}_i\}|}{n} = \frac{3}{5} = 0.6$$

• Set cardinality notation: $|\{i: y_i = \hat{y}_i\}|$

- Set cardinality notation: $|\{i: y_i = \hat{y}_i\}|$
 - Reads as: "Number of indices i such that $y_i = \hat{y}_i$ "

- Set cardinality notation: $|\{i: y_i = \hat{y}_i\}|$
 - Reads as: "Number of indices i such that $y_i = \hat{y}_i$ "
 - Counts how many samples satisfy the condition

- Set cardinality notation: $|\{i: y_i = \hat{y}_i\}|$
 - Reads as: "Number of indices i such that $y_i = \hat{y}_i$ "
 - Counts how many samples satisfy the condition

- Set cardinality notation: $|\{i: y_i = \hat{y}_i\}|$
 - Reads as: "Number of indices i such that $y_i = \hat{y}_i$ "
 - Counts how many samples satisfy the condition

- Set cardinality notation: $|\{i: y_i = \hat{y}_i\}|$
 - Reads as: "Number of indices i such that y_i = ŷ_i"
 - Counts how many samples satisfy the condition
- Alternative: Indicator function notation

Accuracy =
$$\frac{\sum_{i=1}^{n} \mathbf{1}[y_i = \hat{y}_i]}{n}$$

where
$$\mathbf{1}[\text{condition}] = \begin{cases} 1 & \text{if condition is true} \\ 0 & \text{if condition is false} \end{cases}$$

- Set cardinality notation: $|\{i: y_i = \hat{y}_i\}|$
 - Reads as: "Number of indices i such that y_i = ŷ_i"
 - Counts how many samples satisfy the condition
- Alternative: Indicator function notation

Accuracy =
$$\frac{\sum_{i=1}^{n} \mathbf{1}[y_i = \hat{y}_i]}{n}$$

where
$$\mathbf{1}[\text{condition}] = \begin{cases} 1 & \text{if condition is true} \\ 0 & \text{if condition is false} \end{cases}$$

- Set cardinality notation: $|\{i: y_i = \hat{y}_i\}|$
 - Reads as: "Number of indices i such that y_i = ŷ_i"
 - Counts how many samples satisfy the condition
- Alternative: Indicator function notation

Accuracy =
$$\frac{\sum_{i=1}^{n} \mathbf{1}[y_i = \hat{y}_i]}{n}$$

where
$$\mathbf{1}[\text{condition}] = \begin{cases} 1 & \text{if condition is true} \\ 0 & \text{if condition is false} \end{cases}$$

 Both notations are mathematically equivalent and commonly used in ML literature

When Precision/Recall Matter

Cases for this:

Cancer Screening

When Precision/Recall Matter

Cases for this:

- Cancer Screening
- Planet Detection

Precision Metric

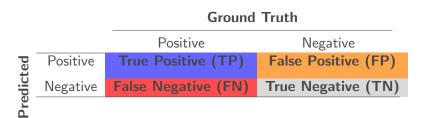
Precision =
$$\frac{|\{i : y_i = \hat{y}_i = \text{Good}\}|}{|\{i : \hat{y}_i = \text{Good}\}|} = \frac{2}{4} = 0.5$$

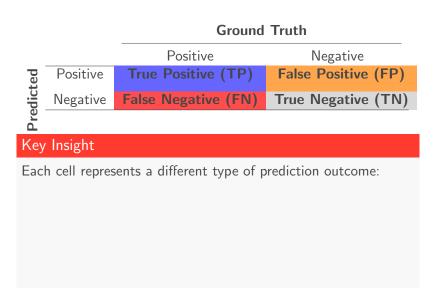
Definition: "The fraction of relevant instances among the retrieved instances"

In simple terms: Out of all times we predict "Good", how many times is it actually "Good"?

Accuracy vs Precision/Recall

$$\label{eq:accuracy} \begin{aligned} \mathsf{Accuracy} &= \frac{98}{100} = 0.98 \\ \mathsf{Recall} &= \frac{0}{1} = 0 \\ \mathsf{Precision} &= \frac{0}{1} = 0 \end{aligned}$$



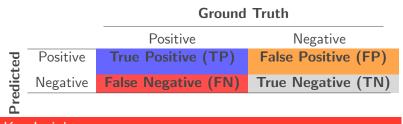




Key Insight

Each cell represents a different type of prediction outcome:

• TP: Correctly predicted positive



Key Insight

Each cell represents a different type of prediction outcome:

- TP: Correctly predicted positive
- FP: Incorrectly predicted positive



Key Insight

Each cell represents a different type of prediction outcome:

- TP: Correctly predicted positive
- FP: Incorrectly predicted positive
- FN: Missed a positive (dangerous!)

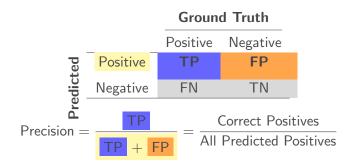


Key Insight

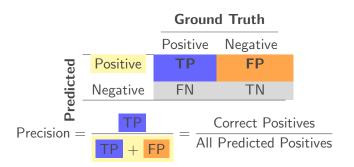
Each cell represents a different type of prediction outcome:

- TP: Correctly predicted positive
- FP: Incorrectly predicted positive
- FN: Missed a positive (dangerous!)
- TN : Correctly predicted negative

Precision: "How accurate are my positive predictions?"



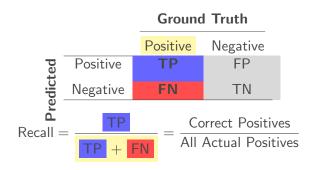
Precision: "How accurate are my positive predictions?"



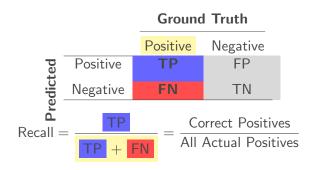
Focus: Look at the PREDICTED POSITIVE ROW

Question: When I predict "positive", how often am I right? **Answer:** Out of all my positive predictions (TP + FP), TP are correct.

Recall: "How many actual positives did I find?"



Recall: "How many actual positives did I find?"



Focus: Look at the ACTUAL POSITIVE COLUMN

 $\mbox{\bf Question:}$ Of all things that ARE positive, how many did I

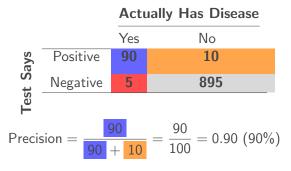
catch?

Answer: Out of all actual positives (TP + FN), I found TP of

them.

		Actually Has Disease		
		Yes	No	
est Says	Positive	90	10	
	Negative	5	895	
ë				

		Actually Has Disease				
		Yes	No			
Says	Positive	90	10			
t S	Negative	5	895			
Precision = $\frac{90}{90 + 10} = \frac{90}{100} = 0.90 (90\%)$						
Recall = $\frac{90}{90 + 5} = \frac{90}{95} = 0.95 (95\%)$						
Accur	$acy = \frac{90}{1}$	+ 895 000	- = 0.985 (98.5%)			



Accuracy =
$$\frac{90 + 895}{1000} = 0.985 (98.5\%)$$

		Actually Has Disease				
		Yes	No			
ays	Positive	90	10			
Test Says	Negative	5	895			
Tes						
Precision = $\frac{90}{90 + 10} = \frac{90}{100} = 0.90 (90\%)$						
Re	call =	0 + 5	$=\frac{90}{95}=0.95\ (95\%)$			
Accur	$acy = \frac{90}{1}$	+ 895 000	$\frac{5}{1} = 0.985 (98.5\%)$			

Mean Error Issues

Is there any downside with using mean error?

Mean Error Issues

Is there any downside with using mean error? Errors can get cancelled out

Pop Quiz: Metrics Choice

Quick Quiz 4

For cancer detection (1 positive case in 1000), which metric is most important?

a) Accuracy only

Answer: b) Recall - we cannot afford to miss cancer cases!

Pop Quiz: Metrics Choice

Quick Quiz 4

For cancer detection (1 positive case in 1000), which metric is most important?

- a) Accuracy only
- b) Recall (finding all cancer cases)

Answer: b) Recall - we cannot afford to miss cancer cases!

Pop Quiz: Metrics Choice

Quick Quiz 4

For cancer detection (1 positive case in 1000), which metric is most important?

- a) Accuracy only
- b) Recall (finding all cancer cases)
- c) Speed of prediction

Answer: b) Recall - we cannot afford to miss cancer cases!

Pop Quiz

Quick Quiz 1

Which metrics should you use for imbalanced datasets?

1. Accuracy only

Answer: c) Precision, recall, and F1-score give a more complete picture!

Pop Quiz

Quick Quiz 1

Which metrics should you use for imbalanced datasets?

- 1. Accuracy only
- 2. Mean squared error

Answer: c) Precision, recall, and F1-score give a more complete picture!

Pop Quiz

Quick Quiz 1

Which metrics should you use for imbalanced datasets?

- 1. Accuracy only
- 2. Mean squared error
- 3. Precision, recall, and F1-score

Answer: c) Precision, recall, and F1-score give a more complete picture!

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

· Features matter:

Choose meaningful features, avoid arbitrary identifiers

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

· Features matter:

Choose meaningful features, avoid arbitrary identifiers

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

Features matter:

Choose meaningful features, avoid arbitrary identifiers

Classification vs Regression:

Discrete outputs vs continuous outputs

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

Features matter:

Choose meaningful features, avoid arbitrary identifiers

Classification vs Regression:

Discrete outputs vs continuous outputs

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

Features matter:

Choose meaningful features, avoid arbitrary identifiers

Classification vs Regression:

Discrete outputs vs continuous outputs

Accuracy isn't everything:

For imbalanced data, use precision, recall, F1-score

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

Features matter:

Choose meaningful features, avoid arbitrary identifiers

Classification vs Regression:

Discrete outputs vs continuous outputs

Accuracy isn't everything:

For imbalanced data, use precision, recall, F1-score

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

Features matter:

Choose meaningful features, avoid arbitrary identifiers

Classification vs Regression:

Discrete outputs vs continuous outputs

Accuracy isn't everything:

For imbalanced data, use precision, recall, F1-score

Visualization is crucial:

Always plot your data first

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

Features matter:

Choose meaningful features, avoid arbitrary identifiers

Classification vs Regression:

Discrete outputs vs continuous outputs

Accuracy isn't everything:

For imbalanced data, use precision, recall, F1-score

Visualization is crucial:

Always plot your data first

ML vs Traditional Programming:

ML learns rules from data, traditional programming uses predefined rules

· Features matter:

Choose meaningful features, avoid arbitrary identifiers

Classification vs Regression:

Discrete outputs vs continuous outputs

Accuracy isn't everything:

For imbalanced data, use precision, recall, F1-score

Visualization is crucial:

Always plot your data first

Use baselines:

Simple baseline models help validate your approach

Summary: Evaluation Metrics

Task	Common Metrics	When to Use
Classification	Accuracy, Precision, Recall, F1	Balanced/Imbalanced data
	Confusion Matrix	Multi-class problems
Regression	MSE, RMSE, MAE	Continuous predictions
	Mean Error	Check for bias

Remember

Choose metrics based on your problem's characteristics and business requirements!